3. CHEMICAL AND PHYSICAL INFORMATION

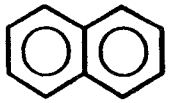
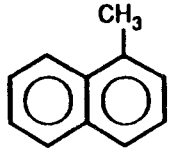
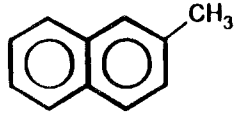
3.1 CHEMICAL IDENTITY

Table 3-l lists common synonyms, trade names and other pertinent identification information for naphthalene, 1-methylnaphthalene, and 2-methylnaphthalene.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 3-2 lists important physical and chemical properties of naphthalene, 1-methylnaphthalene, and 2-methylnaphthalene.

TABLE 3-1. Chemical Identity of Naphthalene, 1-Methylnaphthalene, and 2-Methylnaphthalene

Characteristic	Naphthalene	1-Methylnaphthalene	2-Methylnaphthalene	Reference
Synonym(s)	Tar camphor; albocarbon; naphthene; mothballs; mothflakes; white tar; and others	Alpha-methylnaphthalene; naphthalene, 1-methyl; naphthalene, alpha-methyl	Beta-methylnaphthalene; naphthalene, 2-methyl; naphthalene, beta-methyl	NLM 1995
Registered trade name(s)	Caswell No. 587®	No data	No data	NLM 1995
Chemical formula	$C_{10}H_8$	$C_{11}H_{10}$	$C_{11}H_{10}$	NLM 1995
Chemical structure				
Identification numbers:				
CAS registry	91-20-3	90-12-0	91-57-6	NLM 1995
NIOSH RTECS	QJ0525000	QJ9630000	QJ9635000	HSDB 1995
EPA hazardous waste	U165	No data	No data	NLM 1995
OHM/TADS	7216808	No data	No data	HSDB 1995
DOT/UN/NA/ IMCO shipping	UN1334, UN2304, IMCO 4.1	No data	No data	HSDB 1995 NLM 1995
HSDB	184	5268	5274	NLM 1995
NCI	C52904	No data	No data	NLM 1995

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Naphthalene, 1-Methylnaphthalene, and 2-Methylnaphthalene

Property	Naphthalene	1-Methylnaphthalene	2-Methylnaphthalene	Reference
Molecular weight	128.19	142.20	142.20	Weast et al. 1985
Color	White	Colorless	No data	Verschueren 1983
Physical state	Solid	Liquid	Solid	Verschueren 1983
Melting point	80.5°C	-22°C	34.6°C	Weast et al. 1985
Boiling point	218°C	244.6°C	241°C	Sax and Lewis 1989; Weast et al. 1985
Density	1.145 g/mL	1.0202 g/mL	1.0058 g/mL	Weast et al. 1985
Odor	Strong (tar or mothballs)	No data	No data	HSDB 1995
Odor threshold:				
Water	0.021 mg/L	0.0075 mg/L	0.01 mg/L	Amoore and Hautala 1983; HSDB 1995; Verschueren 1983
Air	0.44 mg/m^3	No data	0.0581-0.2905 mg/m^3	Amoore and Hautala 1983; Ruth 1986
Solubility:				
Water at 20°C	31.7 mg/L	25.8 mg/L	24.6 mg/L at 25°C	HSDB 1995; Mabey et al. 1982
Organic solvent(s)	Soluble in benzene, alcohol, ether, acetone	Soluble in alcohol, ether, benzene	Soluble in alcohol, ether, benzene	Sax and Lewis 1989; Weast et al. 1985
Partition coefficients:				
Log K_{ow}	3.29	3.87	3.86	HSDB 1995; Mabey et al. 1982
Log K_{oc}	2.97	No data	3.39	GDCh 1992; Kenga 1980; Mabey et al. 1982
Vapor pressure	0.087 mmHg	0.054 mmHg	0.068 mmHg	HSDB 1995; Mabey et al. 1982
Henry's law constant	4.6x10^{-4} atm-m^3/mol	3.6x10^{-4} atm-m^3/mol	4.99x10^{-4} atm-m^3/mol	Mabey et al. 1982; Yaws et al. 1991
Autoignition temperature	567°C	529°C	No data	Sax and Lewis 1989
Flashpoint	79°C (open cup)	No data	No data	Sax and Lewis 1989
Flammability limits	0.9% to 5.9%	No data	No data	HSDB 1995
Conversion factors	1 ppm = 5.24 mg/m^3 1 mg/m^3 = 0.191 ppm	1 ppm = 5.91 mg/m^3 1 mg/m^3 = 0.17 ppm	1 ppm = 5.91 mg/m^3 1 mg/m^3 = 0.17 ppm	Verschueren 1983 Verschueren 1983
Explosive limits	No data	No data	No data	